

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 8.99

Global applicability domain: Inside

Local applicability domain index: 7.88e-01

Confidence level: 3.65e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Diphenylamine</div> <div>Measured: 7.64</div> <div>Predicted: 8.73</div>	<div>Image not found</div> <div>Phenacetin</div> <div>Measured: 9.59</div> <div>Predicted: 9.23</div>	<div>Image not found</div> <div>1-Hexadecanol</div> <div>Measured: 9.90</div> <div>Predicted: 9.79</div>
<div>Image not found</div> <div>1-Octadecanol</div> <div>Measured: 10.9</div> <div>Predicted: 10.5</div>	<div>Image not found</div> <div>Methylparaben</div> <div>Measured: 8.57</div> <div>Predicted: 7.06</div>	